The Maximal Eigenvalue of 0-1 Matrices with Prescribed Number of Ones

Shmuel Friedland*

Department of Mathematics
Cornell University
Ithaca, New York 14853
and
California Institute of Technology
Pasadena, California 91125

Dedicated to my teacher Beni Schwarz,
who pioneered the subject 20 years ago.

Submitted by Richard A. Brualdi

ABSTRACT

We determine the maximum spectral radius for 0-1 matrices with $m^2 + l$ ones for $l = 2m, 2m-3$ for all m and for a fixed l and $m > M(l)$. Similar results are obtained for symmetric 0-1 matrix with zero diagonal. In all cases, equality is characterized.

1. INTRODUCTION

Let G be an undirected graph on n vertices with q edges. Then G is represented by an $n \times n$ 0-1 symmetric incidence matrix $A = (a_{ij})_1^n$, having $2q$ ones and zero diagonal. We denote the set of such matrices by $S_{n,2q}$. For $A = (a_{ij}) \in M_n(C)$, let $A^p = (a_{ij}^{(p)})$. For $A \in S_{n,2q}$, $a_{ij}^{(p)}$ gives the number of distinct paths of length p connecting i to j. Assume that G is connected, i.e., A is irreducible. Suppose furthermore that A is primitive. Then $a_{ij}^{(p)} = \rho(A)^p[u_i u_j + O(1)\varepsilon^p]$, for some $0 \leqslant \varepsilon < 1$, where $Au = \rho(A)u$, $u = (u_1, \dots, u_n)^t > 0$, $\sum_{i=1}^n u_i^2 = 1$. Here, $\rho(A)$ denotes the spectral radius of A. It is therefore important to find good upper bounds of $\rho(A)$ in terms of q. Let $M_{n,k}$ be the set of $n \times n$ 0-1 matrices having k ones. Thus any $A \in M_{n,k}$

*On leave from the Hebrew University.

52 Vanderbilt Ave., New York, NY 10017 0024-3795/85/$3.30

represents a directed graph with k edges (we allow the diagonal entries to be one, i.e., our graph can have 1-length cycles). Then, for an irreducible and primitive A we have an analogous formula for $a_{ij}^{(p)}$. In a recent paper Brualdi and Hoffman [1] considered the following maximal problems:

$$\max_{A \in M_{n,k}} \rho(A) = \rho(A_*) = \mu_{n,k}, \tag{1.1}$$

$$\max_{A \in S_{n,2q}} \rho(A) = \rho(B_*) = \sigma_{n,2q}. \tag{1.2}$$

They found the values of $\mu_{n,k}$ and $\sigma_{n,2q}$ in the cases

$$k = m^2, \quad k = m^2 + 1, \qquad 2q = m(m-1).$$

They also characterized the corresponding extremal matrices in these cases. Assume first that $k = m^2$. Then any A_* is permutationally similar to $\operatorname{diag}\{J_m, 0\}$. Here J_m denotes a matrix whose all entries are equal to one. That is, the corresponding maximal graph is the complete directed graph on m vertices. For $2q = m(m-1)$, again the corresponding maximal graph is the complete undirected graph on m vertices. They also showed that for $k = m^2 + 1$ the maximal matrices are obtained by inserting a useless additional 1 anywhere else. Those are only the maximal matrices except for $k = 2,5$. Let E_k be the following $(m+1)\times(m+1)$ matrix:

$$E_k = \begin{pmatrix} J_m & \alpha_p \\ \alpha_q^t & 0 \end{pmatrix}, \qquad k = m^2 + l, \qquad p = \left[\frac{l}{2}\right], \quad q = l - p, \tag{1.3}$$

$$\alpha_q^t = (\alpha_1, \dots, \alpha_m), \qquad \alpha_i = 1, \ i = 1, \dots, q, \quad \alpha_i = 0, \ i = q+1, \dots, m.$$

It is quite tempting to conjecture that E_k is a maximal matrix. That is,

$$\mu_{n,k} = \rho(E_k). \tag{1.4}$$

Indeed, we prove this equality for $k = m^2 + 2m$. Also, we prove (1.4) for

$$k = m^2 + l, \qquad l \geqslant 2, \quad m \geqslant M(l), \tag{1.5}$$

where $M(l)$ is a big enough number. However for $k = m^2 + 2m - 3$ the maximal matrix is

$$H_{m+1}=\begin{pmatrix} & J_{m-1} & & 1 & 1\\ & & & \vdots & \vdots\\ & & & 1 & 1\\ 1 & \cdots & 1 & 0 & 0\\ 1 & \cdots & 1 & 0 & 0\end{pmatrix}. \tag{1.6}$$

In particular, (1.4) is false in general. We also show that H_3 is the exceptional matrix for $k=5$. Let H^0_{m+1} be the matrix obtained from H_{m+1} by replacing the ones on the diagonal with zeros. Then H^0_{m+1} is the maximal matrix for $2q=m^2+m-2$.

These results suggest the following.

CONJECTURE. *Let*

$$k=m^2+l,\quad 2q=m(m-1)+2t,\qquad 1\leqslant l\leqslant 2m,\quad 1\leqslant t<m.$$

Then there exist $(m+1)\times(m+1)$ *matrices* A_* *and* B_* *which satisfy* (1.1) *and* (1.2) *respectively. Moreover, if* A_* *is symmetric, then* B_* *is obtained from* A_* *by replacing the diagonal elements in* A_* *with* 0.

Besides the above mentioned cases, i.e. $l=2m$, $l=2m-3$, we also prove the conjecture in the case (1.5).

We now outline the main ideas and results of our paper. The starting point of our paper and the paper of Brualdi and Hoffman is a fundamental theorem of B. Schwarz [6] which claims that A_* can be chosen so that the elements of each row and column form a decreasing sequence. So A_* is of the form

$$F=\begin{pmatrix} B_1 & A_1\\ A_2 & 0\end{pmatrix},\qquad \text{where}\quad B_1=J_\mu.$$

In Section 2 we obtain upper estimates for $\rho(F)$. Section 3 deals with the asymptotic expansion of $\rho(E_k)$, $k=m^2+l$, $m\to\infty$. In Section 4 we recall some basic inequalities connected with the rearrangement of vectors and prove a key lemma which is needed in the sequel. The computation of the values of $\mu_{n,k}$ in the cases we mentioned above are done in Section 5. Section 6 is devoted to the characterization of the maximal matrices in $M_{n,k}$. The last section is devoted to the class $S_{n,2q}$. Here we combine our methods with the symmetric analog of Schwarz's result given by Brualdi and Hoffman [1].

2. PERTURBATION RESULTS

As usual, let $M_{mn}(C)$ $[M_{mn}(R)]$ and $M_n(C)$ $[M_n(R)]$ denote the set of $m \times n$ complex [real] matrices and the set of $n \times n$ complex [real] matrices respectively. We identify $C^n(R^n)$ with $M_{n1}(C)$ $[M_{n1}(R)]$. For $A \in M_{mn}(C)$ let A^t and A^* denote the transpose and the conjugate transpose of A respectively. For $A \in M_n(C)$ we denote by $|A|$, $\sigma(A)$, and $\rho(A)$ the determinant, spectrum, and spectral radius of A respectively. We now give a sequence of lemmas which are needed in the sequel and may have interest of their own.

LEMMA 1. *Let $A, B \in M_n(C)$. Assume that*

$$\rho(A+B) > \rho(A). \tag{2.1}$$

Then there exists $z \in C$ such that

$$1 \in \sigma\big((zI-A)^{-1}B\big), \qquad |z| > \rho(A). \tag{2.2}$$

Moreover $\rho(A+B)$ is the largest possible $|z|$ for which (2.2) *holds.*

Proof. Let $|\lambda| > \rho(A)$. Then

$$\lambda I - (A+B) = (\lambda I - A)\big[I - (\lambda I - A)^{-1}B\big]. \tag{2.3}$$

As $|\lambda I - A| \neq 0$ for $|\lambda| > \rho(A)$, the determinant of $\lambda I - (A+B)$ vanishes iff (2.2) holds. Clearly $\rho(A+B)$ is the maximum value of $|z|$ which satisfies (2.2). ∎

LEMMA 2. *Let $A, B \in M_n(C)$ be of the form*

$$A = \begin{pmatrix} 0 & A_1 \\ A_2 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} B_1 & 0 \\ 0 & 0 \end{pmatrix},$$

$$A_1, A_2^t \in M_{pq}(C), \quad B_1 \in M_p(C), \quad p+q=n. \tag{2.4}$$

Then the nonzero spectrum of $A+B$ satisfies the equation

$$|\lambda^2 I - \lambda B_1 - A_1 A_2| = 0. \tag{2.5}$$

Proof. Assume that λ is a nonzero eigenvalue of $A + B$. Let $0 \neq (x^t, y^t)^t$ be the corresponding eigenvector of $A + B$. That is, $B_1 x + A_1 y = \lambda x$, $A_2 x = \lambda y$, $\lambda \neq 0$. Clearly $x \neq 0$; otherwise the second equality would imply $y = 0$, which is impossible. So $y = A_2 x/\lambda$, $B_1 x + A_1 A_2 x/\lambda = \lambda x$. That is,

$$\left(\lambda^2 I - \lambda B_1 - A_1 A_2\right) x = 0,$$

and (2.5) is established. ■

In fact, using a similar technique to that in [2, Vol. I, p. 46], one can deduce the identity

$$|\lambda I - (A + B)| = \left|\lambda^2 I - \lambda B_1 - A_1 A_2\right| \lambda^{n-2p}. \tag{2.6}$$

For $B = (b_{ij})$ we denote by B_+ the nonnegative matrix $(|b_{ij}|)$. Recall the Neumann expansion

$$(\lambda I - A)^{-1} = \sum_{k=0}^{\infty} \frac{A^k}{\lambda^{k+1}}, \qquad |\lambda| > \rho(A).$$

So

$$\left[(\lambda I - A)^{-1}\right]_+ \leqslant \sum_{k=0}^{\infty} \frac{A_+^k}{|\lambda|^{k+1}} = (|\lambda| I - A_+)^{-1}, \qquad |\lambda| > \rho(A_+). \tag{2.7}$$

LEMMA 3. *Let the assumptions of Lemma* 1 *hold. Assume in addition that A and B are nonnegative. Then*

$$\rho(r) = \rho\left((rI - A)^{-1} B\right)$$

is a strictly decreasing function on $(\rho(A), \infty)$. *Moreover* $\rho(A + B)$ *is the unique solution of the equation*

$$\rho(r) = 1, \qquad r > \rho(A). \tag{2.8}$$

Proof. Let

$$C(r) = \left(c_{ij}(r)\right) = (rI - A)^{-1} B = \sum_{k=0}^{\infty} \frac{A^k B}{r^{k+1}}, \qquad r > \rho(A).$$

Clearly, either $c_{ij}(r)$ is identically zero or $c_{ij}(r) > 0$ for all $r > \rho(A)$. Let $E = (e_{ij})^n$ be the 0-1 matrix having zeros and ones at the places where $c_{ij}(r)$ is zero and positive respectively.

Assume that E is nilpotent. Then $C(r)$ is nilpotent. So

$$|rI - (A+B)| = |rI - A|\left|I - (rI - A)^{-1}B\right| = |rI - A|, \qquad r > \rho(A).$$

Hence the characteristic polynomials of A and $A+B$ are identical, which contradicts (2.1). According to the Frobenius form (e.g. Gantmacher [2]) there exists a permutation P such that

$$PEP^t = \begin{pmatrix} E_1 & * & \cdots & * \\ 0 & E_2 & \cdots & * \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & E_q \end{pmatrix}, \tag{2.9}$$

where each E_i is either irreducible or the 1×1 zero matrix. Thus, the nonzero spectrum of E comes from $E_{i_1}, \dots, E_{i_s}$. Let $C(r)$ be permuted as in (2.9), and let $C_i(r)$ be the diagonal blocks $i = 1, \dots, q$. As each nonzero entry $c_{ij}(r)$ is strictly decreasing we deduce that $\rho(C_{i_j}(r))$ is a strictly decreasing function on $(\rho(A), \infty)$. Therefore

$$\rho(r) = \max_{1 \leqslant j \leqslant s} \rho\big(C_{i_j}(r)\big)$$

is a strictly decreasing function on $(\rho(A), \infty)$. As $\rho(A+B)$ is an eigenvalue of $A+B$, $\rho(A+B)$ is a solution of (2.8). Since $\rho(r)$ is strictly decreasing, (2.8) has a unique solution for $r > \rho(A)$. ∎

LEMMA 4. *Let the assumption of Lemma* 1 *hold. Assume furthermore that B is a rank one matrix. Then $\rho(A+B)$ is the maximal $|z|$ which satisfies the equation*

$$\operatorname{tr}\left[(zI - A)^{-1}B\right] = 1, \qquad |z| > \rho(A). \tag{2.10}$$

If in addition A and B are nonnegative, then $\rho(A+B)$ is the unique solution of the equation

$$\operatorname{tr}\left[(rI - A)^{-1}B\right] = 1, \qquad r > \rho(A). \tag{2.11}$$

Proof. As $C(\lambda)=(\lambda I - A)^{-1}B$ is also a rank one matrix, then the nonzero eigenvalue of $C(\lambda)$ is given by $\mathrm{tr}(C(\lambda))$. That is,

$$\rho\left[(\lambda I - A)^{-1}B\right] = \left|\mathrm{tr}\left[(\lambda I - A)^{-1}B\right]\right|, \qquad \lambda \notin \sigma(A).$$

Therefore, if A and B are nonnegative, $C(r)$ is a nonnegative matrix for $r > \rho(A)$ and $\rho[(rI - A)^{-1}B] = \mathrm{tr}[(rI - A)^{-1}B]$, $r > \rho(A)$. Hence, according to Lemma 3, $\rho(A+B)$ is the unique solution of (2.11). ■

LEMMA 5. *Let the assumptions of Lemmas 2 and 4 hold. Then $\rho(A+B)$ is the maximal $|z|$ which satisfies the equation*

$$\mathrm{tr}\left[z\left(z^2 I - A_1 A_2\right)^{-1} B_1\right] = 1, \qquad |z|^2 > \rho(A_1 A_2) \tag{2.12}$$

In particular, if A and B are nonnegative, then $\rho(A+B)$ is the unique solution of

$$\mathrm{tr}\left[r\left(r^2 I - A_1 A_2\right)^{-1} B_1\right] = 1, \qquad r^2 > \rho(A_1 A_2). \tag{2.13}$$

Proof. We first note that

$$\rho^2(A) = \rho(A^2) = \rho(A_1 A_2) = \rho(A_2 A_1).$$

Next

$$\left(\lambda^2 I - \lambda B_1 - A_1 A_2\right) = \left(\lambda^2 I - A_1 A_2\right)\left[I - \lambda\left(\lambda^2 I - A_1 A_2\right)^{-1} B\right],$$
$$|\lambda|^2 > \rho(A_1 A_2). \tag{2.14}$$

According to Lemma 2 the eigenvalue λ, $|\lambda| = \rho(A+B)$, satisfies (2.5). Apply now the arguments of the previous lemmas. ■

THEOREM 1. *Let $\|\cdot\|$ be a submultiplicative norm on $M_p(C)$ (i.e. $\|AB\| \leqslant \|A\|\,\|B\|$). Let the assumptions of Lemma 2 hold. Then*

$$\rho(A+B) \leqslant \frac{\|B_1\| + \left(\|B_1\|^2 + 4\|A_1 A_2\|\right)^{1/2}}{2} = \eta(A,B), \tag{2.15}$$

and this inequality is sharp.

Proof. It is well known that for any submultiplicative norm one has the inequality

$$\rho(A) \leqslant \|A\|. \tag{2.16}$$

See for example [3, p. 45]. Hence

$$\rho^2(A) = \rho(A_1A_2) \leqslant \|A_1A_2\|.$$

If $\rho(A+B) \leqslant \rho(A)$, the inequality (2.15) is valid. Therefore we may assume that $\rho(A+B) > \rho(A)$. The equality (2.14) and the obvious modification of Lemma 1 imply that $\rho(A+B)$ is the maximal $|\lambda| > \rho(A)$ such that

$$1 \in \sigma\left[\lambda(\lambda^2 I - A_1A_2)^{-1}B_1\right]. \tag{2.17}$$

The Neumann expansion, the triangle inequality, and the submultiplicativity of $\|\cdot\|$ yield

$$\left\|\lambda(\lambda^2 I - A_1A_2)^{-1}B_1\right\| \leqslant \sum_{k=0}^{\infty} \frac{\|A_1A_2\|^k \|B_1\|}{|\lambda|^{2k+1}}$$

$$= \frac{|\lambda| \|B_1\|}{|\lambda|^2 - \|A_1A_2\|}, \qquad |\lambda|^2 > \|A_1A_2\|.$$

Using the definition of η in (2.15), we deduce the inequality

$$\frac{|\lambda| \|B_1\|}{|\lambda|^2 - \|A_1A_2\|} < 1$$

for $|\lambda| > \eta$. In particular, (2.17) cannot hold for such a λ. Hence we have (2.15). To show that (2.15) sharp we choose $\|\cdot\|$ to be the spectral norm

$$\|A\| = \nu(A) = \rho(A^*A)^{1/2} = \rho(AA^*)^{1/2} \tag{2.18}$$

We then let

$$B_1 = \beta uu^*, \quad \beta > 0, \ u^*u = 1 \qquad [\nu(B_1) = \beta] \tag{2.19}$$

and

$$A_2 = A_1^*, \qquad A_1 A_1^* u = \rho(A_1 A_1^*) u \tag{2.20}$$

So

$$\left[r\left(r^2 I - A_1 A_2\right)^{-1} B_1 \right] u = \frac{r\beta}{r^2 - \rho\left(A_1 A_1^*\right)} u = u \qquad \text{for} \quad r = \eta(A, B).$$

According to (2.17) we have the equality sign in (2.15). ■

We improve the inequality (2.15) in the case that B_1 is a rank one matrix. For $x \in C^n$, denote by $\|x\|$ the standard l_2-norm $\|x\| = (\sum_{i=1}^n |x_i|^2)^{1/2}$.

THEOREM 2. *Let the assumptions of Lemmas* 1 *and* 2 *hold. Assume that* B_1 *is rank* 1 *matrix*

$$B_1 = \beta u v^*, \qquad |\beta| > 0, \quad v^* u = 1. \tag{2.21}$$

Let $r = \xi$ *be the unique positive solution of*

$$|\beta| \sum_{k=0}^{\infty} \frac{\left| v^*(A_1 A_2)^k u \right|}{r^{2k+1}} = 1. \tag{2.22}$$

Then

$$\rho(A + B) \leqslant \xi.$$

Let R *be the largest positive root of the equation*

$$R^3 - aR^2 - bR + c = 0, \tag{2.23}$$

where

$$a = |\beta|, \qquad b = \nu(A_2 A_1), \qquad c = |\beta|\left[\nu(A_2 A_1) - \left\|A_1^* v\right\| \left\|A_2 u\right\|\right]. \tag{2.24}$$

Then

$$\rho(A+B) \leqslant R.$$

Suppose, in addition, that $A_1 A_2$ *is a rank* 1 *matrix*

$$A_1 A_2 = \alpha x y^*, \qquad y^* x = 1. \tag{2.25}$$

Then the above inequality holds, where R *is the largest possible root of the equation* (2.23) *with*

$$a = |\beta|, \qquad b = |\alpha|, \qquad c = |\beta\alpha|\big(1 - |v^* x||y^* u|\big). \tag{2.26}$$

In both cases this inequality is sharp.

Proof. The Neumann expansion yields

$$\left|\operatorname{tr}\left[z\left(z^2 I - A_1 A_2\right)^{-1} B_1\right]\right| = \left|\sum_{k=0}^{\infty} \frac{\operatorname{tr}\left[(A_1 A_2)^k B_1\right]}{z^{2k+1}}\right|$$

$$= \left|\sum_{k=0}^{\infty} \frac{\beta v^*(A_1 A_2)^k u}{z^{2k+1}}\right|$$

$$\leqslant |\beta| \sum_{k=0}^{\infty} \frac{\left|v^*(A_1 A_2)^k u\right|}{r^{2k+1}}, \qquad |z| = r.$$

Note that, since $|\beta| > 0$, the above series is a strictly decreasing function in r on the open interval $(\rho(A), \infty)$. So (2.22) has a unique solution ξ. Since for $r > \xi$, the values of the above series is less than 1, the condition (2.10) does not hold; hence $\rho(A+B) \leqslant \xi$.

We next use the norm inequalities

$$\left|v^*(A_1 A_2)^k u\right| = \left|(A_1^* v)^*(A_2 A_1)^{k-1}(A_2 u)\right|$$

$$\leqslant \|A_1^* v\| \|A_2 u\| \nu(A_2 A_1)^{k-1}, \qquad k \geqslant 1.$$

Therefore

$$\left|\operatorname{tr}\left[z\left(z^2I-A_1A_2\right)^{-1}B_1\right]\right| \leqslant \frac{|\beta|}{r}+\frac{d}{r^3}\sum_{k=0}^{\infty}\frac{\nu(A_2A_1)^k}{r^{2k}}$$

$$=\frac{|\beta|}{r}+\frac{d}{r\left[r^2-\nu(A_2A_1)\right]}$$

$$=\frac{|\beta|\left[r^2-\nu(A_2A_1)\right]+d}{r\left[r^2-\nu(A_2A_1)\right]},$$

$$d=|\beta|\|A_1^*v\|\|A_2u\|$$

Let R be the largest positive root of (2.23). So for $r>R$ the right hand side of the above series will be less than 1. Therefore the condition (2.10) is not satisfied, i.e., $\rho(A+B)\leqslant R$. To see that this inequality is sharp choose $|\beta|=\beta>0$ and

$$A_2u=A_1^*v=z\neq 0, \qquad \nu(A_2A_1)z=(A_2A_1)z. \tag{2.27}$$

This will be the case if

$$v=u\neq 0, \qquad A_2=A_1^*, \qquad A_1A_1^*u=\rho\left(A_1A_1^*\right)u. \tag{2.28}$$

Assume next that A_1A_2 is rank 1 matrix of the form (2.25). Then

$$v^*(A_1A_2)^k u=\alpha^k(v^*x)(y^*u), \qquad k\geqslant 1.$$

Then the inequality $\rho(A+B)\leqslant R$ is deduced as above. Clearly if

$$|\beta|>\alpha\geqslant 0, \qquad (v^*x)(y^*u)\geqslant 0, \tag{2.29}$$

we then deduce that

$$\rho(A+B)=R. \qquad \blacksquare$$

3. ASYMPTOTIC EXPANSIONS

Let $F_{m,p,q}$ be the following $(m+1)\times(m+1)$ matrix:

$$F_{m,p,q}=\begin{pmatrix} J_m & \alpha_p \\ \alpha_q^t & 0 \end{pmatrix}, \qquad 1\leqslant p,q\leqslant m, \tag{3.1}$$

where J_m is the matrix whose all entries are 1 and α_q is defined in (1.3). Clearly $F_{m,p,q}$ satisfies the assumptions of Theorem 2 with

$$B_1 = J_m, \qquad A_1 = \alpha_p, \qquad A_2 = \alpha_q^t,$$

$$A_1 A_2 = \alpha_p \alpha_q^t \qquad \text{(a rank one matrix)}.$$

Then

$$\rho_{m,p,q} = \rho(F_{m,p,q}) \tag{3.2}$$

is the largest positive root of the equation (2.23) with

$$a = m, \qquad b = \min(p,q),$$

$$c = m[\min(p,q)] - pq = \min(p,q)[m - \max(p,q)].$$

The equation (2.23) can be deduced directly. Indeed, the matrix $F_{m,p,q}$ has at most three distinct rows. So its rank is at most 3. Moreover, for $1 \leqslant p, q < m$ these three rows are linearly independent. So, in general, $F_{m,p,q}$ is a rank 3 matrix and the equation (2.23) is its characteristic equation $|RI - F_{m,p,q}| = 0$ divided by R^{m-3}. Since $F_{m,p,q}$ is irreducible and primitive, $\rho_{m,p,q}$ is a simple root of (2.23).

To estimate $\rho_{m,p,q}$ we shall use the fact that $\rho_{m,p,q}$ is the unique positive solution of (2.22). We shall employ the following obvious lemma.

LEMMA 6. *Let f_i be strictly a decreasing function on (a_i, ∞), $i = 1,2$. Assume that*

$$f_1(r) \leqslant f_2(r), \qquad a_2 < r. \tag{3.3}$$

Suppose that

$$f_i(r_i) = 1, \quad a_i < r_i, \qquad i = 1,2.$$

Then

$$r_1 \leqslant r_2. \tag{3.4}$$

Moreover if the inequalities in (3.3) *are strict for $r = r_i$, $i = 1,2$, then the inequalities in* (3.4) *are strict.*

LEMMA 7. *Let m, p, q, s, t be positive integers satisfying*

$$1 \leqslant p, q, s, t \leqslant m, \qquad p + q = s + t, \qquad \min(p, q) < \min(s, t).$$

Then

$$\rho_{m,p,q} < \rho_{m,s,t}. \tag{3.5}$$

Proof. Put

$$f_{m,p,q}(r) = \frac{m}{r} + \frac{pq}{r[r^2 - \min(p, q)]} \tag{3.6}$$

So $\rho_{m,p,q}$ is the unique positive solution $R > \min(p, q)$ satisfying the equation

$$f_{m,p,q}(R) = 1. \tag{3.7}$$

As

$$pq < st, \qquad \min(p, q) < \min(s, t),$$

we easily deduce

$$f_{m,p,q}(r) < f_{m,s,t}(r) \qquad \text{for} \quad r^2 > \min(s, t);$$

then the inequality (3.5) follows from Lemma 6. ∎

LEMMA 8. *Let m, p, q be positive integers satisfying*

$$2 \leqslant m, \qquad 1 \leqslant p, q \leqslant m.$$

Then

$$\rho_{m,p,q} < r_2 = m + \frac{pq}{m^2 - \min(p, q)},$$

$$\rho_{m,p,q} > r_1 = m + \frac{pq}{r_2^2 - \min(p, q)}. \tag{3.8}$$

In particular

$$\rho_{m,p,q} = m\left\{1 + \frac{pq}{m^3}\left[1 + O\left(\frac{1}{m}\right)\right]\right\}. \tag{3.9}$$

Proof. We claim that

$$m < \rho_{m,p,q} < m+1, \qquad 1 \leqslant p, q \leqslant m. \tag{3.10}$$

Indeed, since $F_{m,p,q}$ has at most $(m+1)^2 - 1$ ones, we have the right hand side inequality. Also, as $F_{m,p,q}$ is irreducible for $1 \leqslant p, q$, the spectral radius of $F_{m,p,q}$ is strictly greater than the spectral radius of its principal submatrix J_m. This proves the left hand side inequality of (3.10). So

$$f_{m,p,q}(r) < g(r) = \frac{m}{r} + \frac{pq}{r\left[m^2 - \min(p,q)\right]}, \qquad r > m.$$

As $g(r_2) = 1$, Lemma 6 implies the first inequality of (3.8). In a similar way

$$f_{m,p,q}(r) > h(r) = \frac{m}{r} + \frac{pq}{r\left[r_2^2 - \min(p,q)\right]}, \qquad r < r_2,$$

and Lemma 6 implies the second inequality of (3.8). The expansion (3.9) follows from the inequality

$$\frac{1}{m^2}\left[1 + O\left(\frac{1}{m}\right)\right] = \frac{1}{(m+1)^2} \leqslant \frac{1}{r^2 - \min(p,q)} \leqslant \frac{1}{m^2 - m} = \frac{1}{m^2}\left[1 + O\left(\frac{1}{m}\right)\right]$$

for $m \leqslant r \leqslant m+1$, $1 \leqslant p, q \leqslant m$. ■

4. REARRANGEMENTS

We now recall some basic facts about the rearrangement of vectors. For $u = (u_1, \dots, u_n)^t \in R^n$ we denote by $u_- = (u_1^-, \dots, u_n^-)^t$ a vector Pu for some permutation matrix P such that $\{u_i^-\}$ is a decreasing sequence. For

$u, v \in R^n$ we say that v majorizes u ($u \prec v$) if

$$\sum_{i=1}^{k} u_i^- \leqslant \sum_{i=1}^{k} v_i^-, \qquad k = 1, \dots, n-1,$$

$$\sum_{i=1}^{n} u_i^- = \sum_{i=1}^{n} v_i^-. \tag{4.1}$$

See for example Marshall and Olkin [5] for a good reference on the subject. It is well known (e.g. [5]) that

$$u^t v \leqslant u_-^t v_-, \tag{4.2}$$

and the equality sign holds iff there exist a permutation P such that

$$Pu = u_-, \qquad Pv = v_-. \tag{4.3}$$

In fact, as the set of all u satisfying (4.1) for a fixed v is a convex set spanned by Pv, where P ranges over the set of permutation matrices, we easily deduce a generalization of (4.2).

LEMMA 9. *Let $\alpha, \beta, u, v \in R^n$ be given vectors. Assume that*

$$\alpha \prec u, \qquad \beta \prec v. \tag{4.4}$$

Then

$$\alpha^t \beta \leqslant u_-^t v_-, \tag{4.5}$$

and the equality sign holds iff there exists a permutation matrix such that

$$P\alpha = u_-, \qquad P\beta = v_-. \tag{4.6}$$

LEMMA 10. *Let A_1^t and A_2 be $k \times p$ 0-1 matrices with l_1 and l_2 ones respectively. Denote by e the vector whose all components are* 1. *Put*

$$l_i = s_i p + t_i, \quad 0 \leqslant s_i, \quad 0 \leqslant t_i < p, \qquad i = 1, 2. \tag{4.7}$$

Then

$$e^tA_1A_2e \leqslant w_1^tw_2, \qquad w_i = (\underbrace{p,\dots,p}_{s_i},t_i,0,\dots,0), \quad i=1,2. \tag{4.8}$$

The equality sign holds iff for some permutation matrices P, Q, R

$$PA_1Q = B_1^t, \qquad Q^tA_2R = B_2. \tag{4.9}$$

Here B_i is the matrix in which the first s_i rows equal e^t, the s_i+1st row is of the form

$$(\underbrace{1,\dots,1}_{t_i},0,\dots,0),$$

and the remaining rows contain only zeros.

Proof. It is quite obvious that

$$A_1^te \prec B_1e, \qquad A_2e \prec B_2e.$$

Then the inequality (4.8) follows from (4.5). The equality (4.9) is implied by (4.6). ■

In [4] Katz studied a related maximum problem

$$\max_{A\in M_{n,k}} e^tA^2e.$$

He found the maximal value and characterized the maximal matrices when $k=m^2$ (the solution is $\operatorname{diag}\{J_m,0\}$ up to a permutation) and $k=n^2-l^2$, where $l^2>n^2/2$.

LEMMA 11. *Let $A\in M_n(C)$. Then*

$$\rho(A)\leqslant \nu(A)\leqslant [\operatorname{tr}(AA^*)]^{1/2} = [\operatorname{tr}(A^*A)]^{1/2}. \tag{4.10}$$

The equality sign holds in all inequalities iff αA is a hermitian rank one *matrix for some* $|\alpha| = 1$. *In particular*

$$\rho(A) \leqslant \nu(A) \leqslant \sqrt{k}, \qquad A \in M_{n,k}. \tag{4.11}$$

The equality sign holds in all the inequalities iff $k = m^2$ *and* A *is permutationally similar to* $\operatorname{diag}\{J_m, 0\}$.

Proof. Clearly, we may assume that $A \neq 0$. As AA^* and A^*A are positive definite, all the eigenvalues of AA^* and A^*A are nonnegative. The definition (2.18) implies that

$$\nu(A)^2 \leqslant \operatorname{tr}(AA^*) = \operatorname{tr}(A^*A).$$

The equality holds if AA^* and A^*A have at most one nonzero eigenvalue. So the equality holds iff AA^* and A^*A are rank one matrices. The Cauchy-Binet formula implies that A is a rank one matrix. That is, A is of the form (2.21). Then

$$\rho(A) = |\beta|, \qquad \nu(A) = |\beta| \|u\| \, \|v\|.$$

The Cauchy-Schwarz inequality yields that $\rho(A) = \nu(A)$ iff $v = \gamma u$, $\gamma > 0$. So $A = \bar{\alpha}|\beta|\gamma u u^*$ for some $|\alpha| = 1$.

We next note that

$$\operatorname{tr}(AA^t) = \operatorname{tr}(A^tA) = k, \qquad A \in M_{n,k}.$$

Combine this equality with (4.10) to deduce (4.11). Assume that the equality sign holds in all the inequalities in (4.11). So $A = (a_{ij})$ is a symmetric rank one matrix. That is, $a_{ij} = u_i u_j$. As $a_{ii} = u_i^2$ is either 0 or 1, then u_i is either 0 or 1. Thus $PAP^t = \operatorname{diag}\{J_m, 0\}$ and $k = m^2$. ■

Thus we have shown that

$$\mu_{n,m^2} = m, \tag{4.12}$$

and the maximal matrix A_* is permutationally similar to $\operatorname{diag}\{J_m, 0\}$. This result is proven in [1].

LEMMA 12. *Let the assumptions of Lemma* 2 *hold. Assume furthermore that* $B_1 = J_p$ *and* A_1 *and* A_2 *are* 0-1 *matrices with* l_1 *and* l_2 *zeros respectively.*

Let s_i and t_i be defined as in (4.7). *Denote by R the largest positive root of* (2.23) *where*

$$a = p, \qquad b = (l_1 l_2)^{1/2}, \qquad c = p(l_1 l_1)^{1/2} - (w_1^t w_1)^{1/2}(w_2^t w_2)^{1/2}. \tag{4.13}$$

Then

$$\rho(A+B) \leqslant R.$$

Proof. Lemma 11 yields

$$\nu(A_1 A_2) \leqslant \nu(A_1)\nu(A_2) \leqslant \sqrt{l_1}\sqrt{l_2} = (l_1 l_2)^{1/2}. \tag{4.14}$$

We now apply Theorem 2 to deduce Lemma 12. Indeed,

$$J_p = puu^*, \qquad u = \frac{e}{\sqrt{p}}.$$

So for $k \geqslant 1$

$$\begin{aligned}\beta\left|v^*(A_1A_2)^k u\right| = \left|e^t(A_1A_2)^k e\right| &= \left|\left[(A_1^t e_1)^t (A_2 A_1)\right]^{k-1}(A_2 e)\right| \\ &\leqslant \|A_1^t e_1\| \nu\left[(A_2A_1)^{k-1}\right] \|A_2 e\| \\ &\leqslant (w_1^t w_1)^{1/2} (l_2 l_1)^{(k-1)/2} (w_2^t w_2)^{1/2},\end{aligned}$$

where the last part of the above inequality follows from Lemma 10. ■

5. THE NONSYMMETRIC CASE

We now recall the Schwarz result, which can be stated in this case as follows:

THEOREM 3. *Consider the maximal problem* (1.1). *Then there exists an extremal $A_* = (a_{ij}^*)_1^n$ such that the entries of each row and column of A_* form a decreasing sequence.*

We give a short outline of a proof of this theorem in the next section. Our results are based on the following corollary to Schwarz's theorem.

COROLLARY. *Let* $A_* = (a^*_{ij})_1^n$ *be a solution of* (1.1) *such that each row and column forms a decreasing sequence. Let* μ *be the largest* i *for which* $a^*_{ii} = 1$. *That is,*

$$a^*_{\mu\mu} = 1, \qquad a^*_{(\mu+1)(\mu+1)} = 0. \tag{5.1}$$

Then

$$a^*_{ij} = 1, \quad i, j = 1, \dots, \mu, \qquad a^*_{ij} = 0, \quad i, j = \mu + 1, \dots, n. \tag{5.2}$$

Proof. Since columns μ and $\mu + 1$ of A_* form decreasing sequences, the equality (5.1) implies

$$a^*_{i\mu} = 1, \quad i = 1, \dots, \mu, \qquad a^*_{i(\mu+1)} = 0, \quad i = \mu + 1, \dots, n.$$

As the rows of A_* form decreasing sequences too, we easily deduce (5.2). ∎

The Corollary explains why we studied the spectrum of the matrix $A + B$ satisfying the assumptions of Lemma 2.

THEOREM 4. *Let*

$$k = m^2 + l, \qquad 1 \leqslant l \leqslant 2m.$$

Then

$$\rho(F) \leqslant \frac{m + \sqrt{m^2 + 2l}}{2} \tag{5.3}$$

for any $n \times n$, 0-1 *matrix* F *having* k *ones. The equality sign holds iff* $l = 2m$ *and* F *is permutationally similar to the matrix* $\operatorname{diag}\{E_k, 0\}$. *(Note that* E_k *in this case is symmetric.)*

Proof. According to the Corollary, we may assume that

$$F = \begin{pmatrix} J_\mu & A_1 \\ A_2 & 0 \end{pmatrix}, \qquad A_1, A_2^t \in M_{\mu(n-\mu)}(C). \tag{5.4}$$

Here

$$\operatorname{tr}(A_1A_1^t)=l_1, \qquad \operatorname{tr}(A_2A_2^t)=l_2, \qquad k=\mu^2+l_1+l_2. \tag{5.5}$$

Now Theorem 1 implies

$$\rho(F)\leqslant\frac{\mu+\left[\mu^2+4\nu(A_1A_2)\right]^{1/2}}{2}\leqslant\frac{\mu+\left[\mu^2+4(l_1l_2)^{1/2}\right]^{1/2}}{2}$$
$$\leqslant\frac{\mu+\left[\mu^2+2(l_1+l_2)\right]^{1/2}}{2}\leqslant f(\mu),$$
$$f(\mu)=\frac{\mu+\left[2k-\mu^2\right]^{1/2}}{2}. \tag{5.6}$$

Next we note that

$$2f'(\mu)=1-\mu(2k-\mu^2)^{-1/2}>0, \qquad 0\leqslant\mu<\sqrt{k}.$$

That is, $f(\mu)$ strictly increases in the interval $[0,\sqrt{k}\,]$. As $\mu\leqslant m$,

$$\rho(F)\leqslant f(m),$$

which is the inequality (5.3).

Assume that the equality sign holds in the above inequality. That is, $\mu=m$. Furthermore, in the series (2.22) we must have the equalities

$$|\beta|\left|v^*(A_1A_2)^ku\right|=\left|e^t(A_1A_2)^ke\right|=\|B_1\|\left\|(A_1A_2)^k\right\|$$
$$=\|B_1\|\|A_1A_2\|^k=\|B_1\|\|A_1\|^k\|A_2\|^k$$
$$=m(l_1l_2)^{k/2}=m\left(\frac{l_1+l_2}{2}\right)^k,$$

where $\|A\|=\nu(A)$. In particular

$$e^tA_1A_2e=m(l_1l_2)^{1/2}=m\left(\frac{l_1+l_2}{2}\right).$$

So

$$l_1 = l_2 = s \leqslant m.$$

According to Lemma 10,

$$e^t A_1 A_2 e \leqslant s^2.$$

Hence $s = m$ and the equality sign holds in the above inequality. Lemma 10 implies that $A_1 = A_2^t$ and A_2 has exactly one row of ones. So F is permutationally similar to the matrix given by (1.3). In the next section we shall show that any extremal A_* must be permutationally similar to a matrix F of the form (5.4). ■

THEOREM 5. *Let*

$$k = m^2 + 2m - 3, \qquad m > 1. \tag{5.7}$$

Then

$$\rho(F) \leqslant \frac{m - 1 + (m^2 + 6m - 7)^{1/2}}{2} \tag{5.8}$$

for any $n \times n$, 0-1 *matrix* F *having* k *ones. For* $m > 2$ *the equality sign holds iff* F *is permutationally similar to* $\operatorname{diag}\{H_{m+1}, 0\}$, *where* H_{m+1} *is given by* (1.6).

Proof. We first note that the right hand side of (5.8) is equal to $f(m-1)$. Assume that F is of the form (5.4). We now use the arguments given in the proof of Theorem 4. First, if $\mu < m - 1$, we have strict inequality in (5.8). Second, if $\mu = m - 1$ and the equality sign holds in (5.8), we deduce that

$$l_1 = l_2 = 2(m-1), \qquad e^t A_1 A_2 e = m[2(m-1)].$$

According to Lemma 10, we may assume, after a suitable permutation of rows and columns, that A_1 and A_2^t have the first two columns consisting entirely of ones. That is, F is $\operatorname{diag}\{H_{m+1}, 0\}$.

In that case, F is a rank 2 matrix whose spectral radius ρ satisfies the quadratic equation

$$\rho^2 - (m-1)\rho - 2(m-1) = 0. \tag{5.9}$$

So we have the equality sign in (5.8).

Assume next that F is of the form (5.4) with $\mu = m$. Lemma 12 implies that $\rho(F)$ is bounded from above by $0 < R$ which solves the equation

$$\frac{m}{R} + \frac{(m-1)(m-2)}{R\{R^2 - [(m-1)(m-2)]^{1/2}\}} = 1.$$

Clearly, if $m = 2$ then $R = \rho = 2$. Assume that $m > 2$.

Lemma 6 yields that $\rho(F) < R$ if R is the positive solution of

$$\frac{m}{R} + \frac{(m-1)(m-2)}{R[R^2 - (m-1)]} = 1.$$

We claim that $R = \rho$. Indeed, (5.9) is equivalent to

$$\rho^2 - (m-1) = (m-1)(\rho+1).$$

So

$$\begin{aligned}\frac{m}{\rho} + \frac{(m-1)(m-2)}{\rho[\rho^2 - (m-1)]} &= \frac{m}{\rho} + \frac{(m-2)}{\rho(\rho+1)}\\ &= \frac{m(\rho+1) + m - 2}{\rho(\rho+1)} = \frac{(m-1)\rho + \rho + 2(m-1)}{\rho(\rho+1)}\\ &= \frac{\rho^2 - 2(m-1) + \rho + 2(m-1)}{\rho(\rho+1)} = 1.\end{aligned}$$

This proves the inequality (5.8). The equality case will be discussed in the next section. ■

THEOREM 6. *Let k and m satisfy the assumptions of Theorem 4. Assume that F is an extremal matrix to the problem (1.1) of the form (5.4). Then*

$$m - \sqrt{l} < \mu \tag{5.10}$$

unless $l = 1$ *and* $m = 1,2$. *In particular,*

$$\rho(A) \leqslant m \qquad \text{for} \quad A \in M_{n, m^2+1}, \tag{5.11}$$

and the equality sign holds if either A *has* J_m *as its principal submatrix, or* $k = 2$ *or* 5 *and* A *is permutationally similar respectively to*

$$\operatorname{diag}\left\{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, 0\right\} \quad \text{or} \quad \operatorname{diag}\{H_3, 0\}.$$

Proof. Theorem 4 implies that it is enough to consider the case

$$1 \leqslant l \leqslant 2m - 1. \tag{5.12}$$

Let F be of the form (5.4). In the proof of Theorem 4 we showed that

$$\rho(F) \leqslant f(\mu),$$

where $f(\mu)$ is given in (5.6). A straightforward calculation shows that

$$f(\mu) \leqslant m \qquad \text{for} \quad \mu \leqslant m - \sqrt{l}\,.$$

Suppose first that $l \geqslant 2$. Then

$$\rho(F) \geqslant \rho(E_k) \geqslant \rho(E_{m^2+2}) > m.$$

Therefore we have the inequality (5.10). Assume now that $l = 1$. Clearly $\rho(F) \geqslant m$. Thus, if $\rho(F) > m$ we must have the inequality $\mu > m - \sqrt{l} = m - 1$. So $\mu = m$. But then, either A_1 or A_2 is a zero matrix and

$$\rho(F) = \rho(J_m) = m.$$

This establishes the inequality (5.11). The equality case will be discussed in the next section. ∎

THEOREM 7. *Let* $l \geqslant 2$ *be fixed. Then there exists* $M = M(l)$ *such that for* $m \geqslant M(l)$ *any maximal solution* A_* *to the problem* (1.1) *is permutationally similar either to* $\operatorname{diag}\{E_k, 0\}$ *or to* $\operatorname{diag}\{E_k^t, 0\}$.

Proof. Choose m to satisfy the inequality

$$m \geqslant 2l + \sqrt{l}\,. \tag{5.13}$$

Let F be an extremal matrix of the form (5.4). By Theorem 6 the inequality (5.10) holds.

Assume that A_1 and A_2 have l_1 and l_2 ones. So

$$l_1 + l_2 = k - \mu^2 = 2\mu(m-\mu) + (m-\mu)^2 + l < 2\mu(m-\mu) + 2l$$

in view of the inequality (5.10). Put

$$l_i = s_i\mu + t_i, \quad 0 \leqslant t_i < \mu, \qquad i = 1,2. \tag{5.14}$$

Then the inequalities (5.13) and (5.10) yield

$$s_1 + s_2 \leqslant 2(m-\mu). \tag{5.15}$$

Using Lemma 10, we get

$$e^t A_1 A_2 e \leqslant (m-\mu)\mu^2 + \tau_1\tau_2,$$

$$\tau_1 = \left[\frac{(m-\mu)^2 + l}{2}\right], \qquad \tau_2 = (m-\mu)^2 + l - \tau_1. \tag{5.16}$$

The equality sign holds for A_i as described in Lemma 10 with l_1 and l_2 of the form

$$l_i = (m-\mu)\mu + \tau_i, \quad i = 1,2 \quad \text{or} \quad l_i = (m-\mu)\mu + \tau_{3-i}, \quad i = 1,2. \tag{5.17}$$

Also

$$\|A_1^t e\|\|A_2 e\| \leqslant \frac{\|A_1^t e\|^2 + \|A_2 e\|^2}{2}$$

$$\leqslant \frac{s_1\mu^2 + t_1^2 + s_2\mu^2 + t_2^2}{2} \leqslant (m-\mu)\mu^2 + 2l^2.$$

Next we estimate the series (2.22):

$$\sum_{k=0}^{\infty} \frac{e^t(A_1A_2)^k e}{r^{2k+1}} \leqslant \frac{\mu}{r} + \frac{e^t(A_1A_2)e}{r^3} + \sum_{k=2}^{\infty} \frac{\|A_1^t e\|\|A_2 e\|\|A_2A_1\|^{k-1}}{r^{2k+1}}$$

$$\leqslant \frac{\mu}{r} + \frac{e^t(A_1A_2)e}{r^3} + \frac{\|A_1^t e\|\|A_2 e\|\|A_2A_1\|}{r^3\left(r^2 - \|A_2A_1\|\right)}$$

$$\leqslant \frac{\mu}{r} + \frac{e^t(A_1A_2)e}{r^3} + \frac{\left[(m-\mu)\mu^2 + 2l^2\right](l_1l_2)^{1/2}}{r^3\left[r^2 - (l_1l_2)^{1/2}\right]}.$$

Then for $r \geqslant m$ the above series are majorized by

$$g(r) = \frac{\mu}{r} + \frac{e^t(A_1A_2)e}{rm^2} + \frac{\left[(m-\mu)\mu^2 + 2l^2\right](l_1l_2)^{1/2}}{rm^2\left[m^2 - (l_1l_2)^{1/2}\right]}$$

Thus, if $\rho(F) > m$, we deduce from Lemma 6

$$\rho(F) \leqslant \mu + \frac{e^t(A_1A_2)e}{m^2} + \frac{\left[(m-\mu)\mu^2 + 2l^2\right](l_1l_2)^{1/2}}{m^2\left[m^2 - (l_1l_2)^{1/2}\right]} \tag{5.18}$$

Let $\mu = m - s$, $1 \leqslant s < \sqrt{l}$. As

$$(l_1l_2)^{1/2} \leqslant \frac{l_1 + l_2}{2} \leqslant \mu(m-\mu) + l = (m-s)s + l,$$

$$m^2 - (l_1l_2)^{1/2} \geqslant m^2 - (m-s)s - l,$$

$$e^t A_1 A_2 e \leqslant s(m-s)^2 + l^2,$$

we get

$$\rho(F) \leqslant m - s + \frac{s(m-s)^2 + l^2}{m^2} + \frac{\left[s(m-s)^2 + 2l^2\right]\left[(m-s)s + l\right]}{m^2\left[m^2 - (m-s)s - l\right]}$$

$$= m - \frac{s^2}{m} + O\left(\frac{1}{m^2}\right).$$

So for big enough m we get that $\rho(F) < m$, which contradicts our assumptions. Thus $s = 0$. In that case (5.18) yields

$$\rho(F) \leqslant m + \frac{e^t A_1 A_2 e}{m^2} + O\left(\frac{1}{m^4}\right).$$

In view of (5.16)

$$\rho(F) \leqslant m + \frac{[l/2](l-[l/2])}{m^2} + O\left(\frac{1}{m^4}\right), \tag{5.19}$$

and the equality sign can hold only if A_1 and A_2^t have the same nonzero column, which have $\tau_1 = [l/2]$ ones in common. So F is permutationally similar either to $\operatorname{diag}\{E_k, 0\}$ or to $\operatorname{diag}\{E_k^t, 0\}$. Finally, use (3.9) to deduce the equality sign in (5.19) for $\operatorname{diag}\{E_k, 0\}$ and $\operatorname{diag}\{E_k^t, 0\}$. Thus we have proved the theorem for a matrix F of the form (5.4). The equality case for an arbitrary F is discussed in the next section. ■

6. THE EQUALITY CASE

A matrix E is called reducible if E is permutationally similar to a matrix of the form (2.9) with $q \geqslant 2$. The matrices E_i are called the components of E. Otherwise E is called irreducible. E is called completely reducible if the matrix given by (2.9) is block diagonal and each E_i is either an irreducible matrix or the 1×1 zero matrix.

LEMMA 13. *Let*

$$m^2 + 1 \leqslant k \leqslant (m+1)^2. \tag{6.1}$$

Then

$$m = \mu_{n, m^2+1} < \mu_{n, m^2+2} < \cdots < \mu_{n,(m+1)^2} = m + 1. \tag{6.2}$$

Moreover for $k \geqslant m^2 + 2$ any extremal A_* is either irreducible or permutationally similar to a matrix $\operatorname{diag}\{E, 0\}$ *where E is an irreducible matrix.*

Proof. We first note that $n \geqslant m + 1$. Also the equalities

$$m = \mu_{n, m^2+1}, \qquad \mu_{n,(m+1)^2} = m + 1$$

were established before. Let $k = m^2 + 2$. Then

$$\mu_{n,m^2+2} \geqslant \rho(E_{m^2+2}) > m.$$

Assume that A_* is reducible. So

$$\rho(A_*) = \rho(E)$$

for some component of A_*. If E does not have $m^2 + 2$ ones, then

$$\rho(A_*) = \rho(E) \leqslant \mu_{n,m^2+1} = m,$$

which is impossible. So E has $m^2 + 2$ ones, and hence A_* is permutationally similar to $\operatorname{diag}\{E, 0\}$. In case A_* is irreducible, we let $E = A_*$. Then E is an $l \times l$ matrix with $l \geqslant m + 1$. Let $G \in M_{l,1}$ and the nonzero entry of G be situated in a place where E has a zero entry. As E is irreducible, we have the inequality

$$\mu_{n,m^2+2} = \rho(E) < \rho(E + G) \leqslant \mu_{n,m^2+3} = \rho(B_*).$$

See for example [2, Vol. II, Chapter 13].

As before, we deduce that either B_* is irreducible or B_* is permutationally similar to $\operatorname{diag}\{E, 0\}$ whose E is irreducible. Continuing in the same manner, we prove the lemma. ∎

We now recall the basic ingredient in the Schwarz theorem [6].

LEMMA 14. *Let E be an $l \times l$ nonnegative irreducible matrix with the rows $e_1^t, \ldots, e_n^t$, such that*

$$Eu = \rho(E)u, \qquad u > 0, \quad u = u_-. \tag{6.3}$$

Denote by E_- the matrix with the rows $(e_1)_-^t, \ldots, (e_n)_-^t$, i.e., the ith row of E_- is the ith row of E rearranged in decreasing order. Then

$$\rho(E) \leqslant \rho(E_-). \tag{6.4}$$

If E_- is also irreducible, then the equality sign holds iff

$$(e_i^t)u = (e_i^t)_- u, \qquad i = 1, \ldots, n. \tag{6.5}$$

We give a short proof of this fact for the reader's convenience.

Proof. As

$$(e_i^t)u \leqslant (e_i^t)_- u_- = (e_i^t)_- u,$$

we deduce that

$$E_- u \geqslant \rho(E)u.$$

Since $u > 0$, we get the inequality (6.4) even if E_- is reducible. If E_- is irreducible and the equality sign holds in (6.4), then

$$E_- u = \rho(E)u.$$

See for example [2, Vol. II, Chapter 13]. So we have the equalities (6.5). Vice versa, if the equalities (6.5) hold, we deduce the above equality. Since E_- is irreducible and $u > 0$, we deduce the equality $\rho(E_-) = \rho(E)$. ∎

Assume that E_- is irreducible. Then

$$(E_-)^t v = \rho(E_-)v, \qquad v > 0. \tag{6.6}$$

It is quite easy to prove, using the above equality, that $v = v_-$. Put

$$F = \left[(E_-)^t\right]_-; \tag{6.7}$$

then according to Lemma 14

$$\rho(F) \geqslant \rho\left[(E_-)^t\right] = \rho(E_-) \geqslant \rho(E). \tag{6.8}$$

Moreover, Schwarz proves that the elements of each row and column of F form a decreasing sequence.

Proof of the equality case in Theorem 4. Assume that $l = 2m$. Suppose that

$$\rho(A_*) = \frac{m + (m^2 + 4m)^{1/2}}{2}.$$

Then according to Lemma 13, A_* is permutationally similar to $\operatorname{diag}\{G, 0\}$

and G is irreducible. We may assume that G satisfies the assumptions of Lemma 14 (otherwise consider PGP^t for some permutation matrix P). Then G_- is also an extremal matrix. Therefore G_- is irreducible and we have the equality case in Lemma 14.

Let $E=(G_-)^t$. Again E is irreducible and extremal, Put $F=E_-$. As before, F is extremal and irreducible. According to Theorem 4, $F=E_k$, $k=m^2+2m$. Let $u=(u_1,\dots,u_{m+1})^t>0$ be the eigenvector of E_k. Clearly

$$u_1=\cdots=u_m>u_{m+1},$$

hence the equalities (6.5) imply that $E=E_-=E_k$. So $G_-=E_k$ and therefore $G=E_k$. ■

Proof of the equality case in Theorem 5. Assume that $m>2$. Then $l=2m-3>1$ and we repeat the arguments of the equality case in Theorem 4. For $m=2$ we get $k=5=2^2+1$ and the equality cases discussed below. ■

Proof of the equality case in Theorem 6. Assume that

$$\rho(A_*)=m, \qquad A_*\in M_{n,\,m^2+1}.$$

Assume first that A_* is reducible but not completely reducible. So

$$m=\rho(A_*)=\rho(E),$$

where E is some irreducible component of A_*. Since E is irreducible, Lemma 11 implies that $E=J_m$. In that case A_* has J_m as its principal submatrix. Assume next that A_* is completely reducible and J_m is not its component. The arguments above show that A_* has only one nontrivial component E such that

$$m=\rho(E), \qquad E\in M_{l,\,m^2+1}$$

and E is irreducible. Again we may assume that E satisfies the assumptions of Lemma 14. Consider E_-. Assume first that E_- is reducible but not completely reducible. So E contains J_m as its principal submatrix. That is, E_- has at most $m+1$ nonzero rows. Since E is irreducible, E is an $(m+1)\times(m+1)$ matrix. Since E_- has exactly m^2+1 ones and E_- has J_m as its principal submatrix, then either E_- has a zero row or E_- has m rows with m ones and one row i with a one in the first column. Since E is irreducible, E (and E_-)

cannot have a zero row. So we are left with the second possibility. Assume that $m = 1$. Then

$$E_- = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix},$$

and the only irreducible corresponding matrix is

$$E = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Suppose $m > 1$. Then all rows of E_- except the ith row are of the form $(1,\dots,1,0,\dots,0)$.

The assumption that J_m is a principal submatrix of E_- implies that $i = m+1$. From the proof of Lemma 14 it follows that

$$E_- u \geqslant mu, \qquad u = u_- > 0;$$

therefore

$$u_1 = \cdots = u_m, \qquad u_1 \geqslant mu_{m+1} > 0.$$

But then we can never get the equality

$$Eu = mu$$

for an irreducible E. We now assume that E_- is completely reducible. Then E_- is permutationally similar to $\operatorname{diag}\{J_m, 1\}$. So E_- has one row with one nonzero element. As $m > 1$, we have a contradiction as before.

Finally we shall assume that E_- is also irreducible. Let $F = [(E_-)^t]_-$. Again it is enough to assume that F is irreducible. So F is of the form (5.4). Therefore $\mu = m - 1$ and $\rho(F) = f(m-1)$. From the proof of Theorem 5 it follows that $F = H_{m+1}$. But then $m = 2$. As before, we can show that $E = F$. ■

Proof of the equality case in Theorem 7. Let $m \geqslant M(l)$, $l \geqslant 2$. Assume that

$$\rho(A_*) = \rho(E_k), \qquad k = m^2 + l.$$

According to Lemma 13, A_* is permutationally similar to $\operatorname{diag}\{E,0\}$ where $E \in M_{j,k}$ is irreducible. We may assume that E satisfies the assumptions of Lemma 14. Then E_- is also extremal and is irreducible or completely reducible. In the second case E_- is permutationally similar to $\operatorname{diag}\{E_1, 0\}$. So E_- and E have a zero row. That is, E is reducible, and we contradicted our assumptions. So E_- is also irreducible. Thus $F = [(E_-)^t]_-$ is irreducible and of the form (5.4). Therefore F is either E_k or E_k^t. In particular, E is an $(m+1)\times(m+1)$ matrix. Let

$$Fu = \rho(F)u, \qquad u = (u_1, \dots, u_{m+1}), \quad u_1 \geqslant u_2 \geqslant \cdots \geqslant u_{m+1} > 0.$$

Since u is unique, according to the proof of Lemma 14

$$Gu = \rho(G)u, \qquad \rho(G) = \rho(F), \qquad G = (E_-)^t.$$

Assume first that $F = E_k$. Then

$$u_1 = \cdots = u_p > u_{p+1} = \cdots = u_m > u_{m+1}, \qquad p = \left[\frac{l}{2}\right].$$

Then the equalities (6.5) imply that $F = G$. The same arguments apply if $F = E_k^t$. Thus E_- is either E_k or E_k^t, and as before we deduce that $E = E_-$. ∎

The inequality (5.11) and the equality case are proven in [1]. However, as the methods in [1] differ from ours, we decided to give our proof for the sake of completeness.

7. THE SYMMETRIC CASE

Denote by $S_{n,k}$ the set of 0-1 $n \times n$ symmetric matrices with $k = 2t$ ones and zero diagonal. Let $S_{n,k}^*$ be the subset of $S_{n,k}$ consisting of those matrices $A = (a_{ij})$ such that whenever $i < j$ and $a_{ij} = 1$, then $a_{kl} = 1$ for all $k < l$ with $k \leqslant i$ and $l \leqslant j$. Recently, Brualdi and Hoffman [1] established the precise symmetric analog of Schwarz's result [6]. Note that in the symmetric case the maximal matrix must have the monotone property. This is contrary to the nonsymmetric case (e.g., [6]).

THEOREM 8 (Brualdi, Hoffman). *Let*

$$\max_{A \in S_{n,k}} \rho(A) = \rho(B_*) = \sigma_{n,k}. \tag{7.1}$$

Then $PB_*P^t \in S_{n,k}^*$ for some permutation P.

Assume that $B_* = (b_{ij}^*) \in S_{n,k}^*$. By considering the maximal p such that $b_{p(p+1)}^* = 1$, we deduce that B^* is of the form

$$A = \begin{pmatrix} J_\mu - I_\mu & A_1 \\ A_1^t & 0 \end{pmatrix}. \tag{7.2}$$

Here by I_p we mean the $p \times p$ identity matrix. As

$$\nu(J_\mu - I_\mu) = \mu - 1, \tag{7.3}$$

Theorem 1 and the inequality (4.11) imply

$$\rho(A) \leqslant \frac{(\mu-1)+(2k-\mu^2+1)^{1/2}}{2} = g(\mu). \tag{7.4}$$

As $g(x)$ is a strictly increasing function on $\left[0, \sqrt{k+\frac{1}{2}}\,\right]$, the maximal value of the right hand side of (7.4) is achieved either for $\mu = m-1$ or $\mu = m$. Comparing these two values, we deduce

THEOREM 9. *Let*

$$k = m(m-1)+l, \qquad 0 \leqslant l = 2t < 2m. \tag{7.5}$$

Then for any $A \in S_{n,k}$

$$\rho(A) \leqslant \frac{m-1+\left[(m-1)^2+2l\right]^{1/2}}{2}. \tag{7.6}$$

For $l = 0$ the equality sign holds iff A is permutationally similar to the matrix

$$\operatorname{diag}\{J_m - I_m, 0\}.$$

REMARK. For $l = 0$, this result is due to Brualdi and Hoffman [1].

We now state a version of Theorem 2 which is needed here.

THEOREM 10. *Let A and B be real nonnegative matrices of the form (2.4). Assume furthermore that*

$$B_1 = \beta u v^t - \gamma I, \qquad u, v \geqslant 0, \quad v^t u = 1, \quad \beta > \gamma > 0. \tag{7.7}$$

Then $\rho(A+B)$ *is the unique positive solution of*

$$\sum_{k=0}^{\infty} \beta \frac{v^t(A_1A_2)^k u}{r^k(r+\gamma)^{k+1}} = 1. \tag{7.8}$$

Moreover, if

$$v = u > 0, \qquad A_2 = A_1^t, \qquad A_1A_1^t u = \omega u, \tag{7.9}$$

then the equality sign holds in (2.15), *where* $\|\cdot\|$ *is the spectral norm.*

Proof. Let $r = \rho(A+B)$. Lemma 2 and (7.7) imply that

$$|r(r+\gamma)I - r\beta uv^t - A_1A_2| = 0.$$

Note that

$$r \geqslant \rho(B_1) = \beta - \gamma > 0, \qquad r \geqslant \rho(A).$$

Hence r satisfies the equation

$$\left| I - \left(I - \frac{A_1A_2}{r(r+\gamma)} \right)^{-1} \frac{\beta uv^t}{r+\gamma} \right| = 0.$$

As in the proof of Theorem 2, we deduce that r satisfies the equation (7.8). Assume next that (7.9) holds. As $u > 0$, it follows that $\omega = \rho^2(A)$. Also $\nu(B_1) = \beta - \gamma$. Summing the series in (7.8), we get the equation

$$\frac{\beta r}{r(r+\gamma) - \omega} = 1.$$

So the equality sign holds in (2.15). ∎

THEOREM 11. *Let*

$$k = m(m-1) + 2m - 2, \qquad m \geqslant 2. \tag{7.10}$$

Then for any $A \in S_{n,k}$

$$\rho(A) \leqslant \frac{m-2+(m^2+4m-4)^{1/2}}{2}. \tag{7.11}$$

The equality sign holds iff A is permutationally similar to diag$\{H^0_{m+1},0\}$, *where* H^0_{m+1} *is obtained from* H_{m+1} *(given by* (1.6)*) upon replacing its diagonal by the zero diagonal.*

Proof. As in the proof of Theorem 5, it is left to consider the case $\mu = m$. As

$$\nu(A_1A_1^t) \leqslant l = m-1, \qquad \|A_1^t e\| \leqslant (m-1)^{1/2},$$

from Theorem 10 we obtain that $\rho(A) \leqslant R$, where R is the unique positive solution of

$$\frac{m}{R+1} + \frac{m-1}{[R(R+1)-(m-1)](R+1)} = 1. \tag{7.12}$$

Note that the right hand side of (7.11) satisfies the equation

$$(m-1)r = r(r+1) - 2(m-1). \tag{7.13}$$

So

$$\begin{aligned}\frac{m}{r+1} + \frac{(m-1)}{[r(r+1)-(m-1)](r+1)} &= \frac{m}{r+1} + \frac{1}{(r+1)^2}\\ &= \frac{m(r+1)+1}{r(r+1)+r+1}\\ &= \frac{mr+m+1}{mr+2m-1} < 1\end{aligned}$$

for $m > 2$. So $\rho(A) \leqslant R < r$ for $m > 2$.

Assume that A is of the form (7.2), $\mu = m-1$, and $\rho(A) = r$. It then follows that

$$\|A_1^t e\|^2 = 2(m-1)^2.$$

Lemma 10 implies that A_1^t has precisely two rows of ones. That is, A is permutationally similar to diag$\{H^0_{m+1},0\}$. Assume finally that $m=2$. Then $k=4$, and the only matrix in $S^*_{n,4}$ is the matrix diag$\{H^0_3,0\}$. ∎

We state the symmetric analog of Theorem 7. Denote by E_k^0 the matrix obtained from E_k by replacing its diagonal with the zero diagonal.

THEOREM 12. *Let $l = 2t \geqslant 2$ be fixed. Then there exists $M(l)$ such that for $m \geqslant M(l)$ any maximal solution B_* to the problem* (1.2) *is permutationally similar to* $\operatorname{diag}\{E_k^0, 0\}$.

Proof. As $\rho(B_*) > m-1$, the inequality (7.4) yields

$$m - \mu - \tfrac{1}{2} < \left(l + \tfrac{1}{4}\right)^{1/2}.$$

Estimating from above the series (7.8), we deduce that the positive solution r of

$$\frac{\mu}{r+1} + \frac{e^t A_1 A_1^t e}{(r+1)[r(r+1) - l_1]} = 1 \tag{7.14}$$

majorizes $\rho(B_*)$. Here l_1 is the number of ones in A_1. Recall that

$$2l_1 = k - \mu^2 + \mu = (m-\mu)(m+\mu-1) + 2t.$$

Put $\mu = m - s$. Then

$$2l_1 = s(2m - s - 1) + 2t = 2s(m-s) + s(s-1) + 2t.$$

So, for a big enough m, Lemma 10 yields

$$eA_1A_1^t e \leqslant s(m-s)^2 + \left[t + \frac{s(s-1)}{2}\right]^2.$$

Let R be the positive solution of

$$\frac{m-s}{R+1} + \frac{s(m-s)^2 + [t + s(s-1)/2]^2}{(R+1)[R(R+1) - t - s(m-s) - s(s-1)/2]} = 1. \tag{7.15}$$

Consider first the case $s = 0$. Then Theorem 10 yields that $R = \rho(E_k^0)$. Moreover, Lemma 10 implies that $\rho(B) = R$ iff B is permutationally similar to $\operatorname{diag}\{E_k^0, 0\}$.

As in Section 3, we deduce that

$$R=\rho\left(E_k^0\right)=m-1+\frac{t^2}{m^2}+O\left(\frac{1}{m^3}\right). \tag{7.16}$$

So

$$\rho\left(E_k^0\right)\left[\rho\left(E_k^0\right)+1\right]\geqslant m(m-1)+\frac{2t^2}{m}+O\left(\frac{1}{m^2}\right).$$

We claim that

$$\frac{m}{R+1}+\frac{t^2}{(R+1)[R(R+1)-t]}$$
$$>\frac{m-s}{R+1}+\frac{s(m-s)^2+[t+s(s-1)/2]^2}{(R+1)[R(R+1)-t-s(m-s)-s(s-1)/2]}$$

for $s\geqslant 2$.

Indeed, let

$$x=R(R+1)-t.$$

Hence, it is enough to show that

$$\frac{sx+t^2}{x}>\frac{u}{x-v}\qquad\text{for}\quad x=m(m-1)-t+\frac{2t^2}{m}+O\left(\frac{1}{m^2}\right),$$

where

$$u=s(m-s)^2+\left[t+\frac{s(s-1)}{2}\right]^2,\qquad v=s(m-s)+\frac{s(s-1)}{2}.$$

The above inequality holds for

$$x>\xi=\frac{sv+u-t^2+\left[(sv+u-t^2)^2+4t^2sv\right]^{1/2}}{2s}.$$

Expanding the square root in a Maclaurin series, we obtain

$$\xi=\frac{sv+u-t^2}{s}+O\left(\frac{1}{m}\right). \tag{7.17}$$

As

$$\frac{sv+u-t^2}{s} = (m-s)m + \frac{s(s-1)}{2} + \frac{[t+s(s-1)/2]^2 - t^2}{s}.$$
$$= (m-1)m - (s-1)m + O(1),$$

we have established the theorem for $s \geqslant 2$. Assume that $s = 1$. If A_1 has one column of ones, then B_* has $J_m - I_m$ as its principal submatrix and we are back in the case $s = 0$. Assume finally that each column of A_1 has at most $m-2$ ones. As in Lemma 10, we deduce

$$eA_1A_1^te \leqslant (m-2)^2 + (t+1)^2$$

for m big enough. Using the above arguments, we get the equality (7.17) with

$$s = 1, \qquad v = m-1, \qquad u = (m-2)^2 + (t+1)^2.$$

So

$$\xi = v + u - t^2 + O\left(\frac{1}{m}\right) = (m-1) + (m-2)^2 + O(1) = m(m-3) + O(1)$$
$$< m(m-1) + O(1),$$

and the theorem is proved in this case too. ∎

I would like to thank Binyamin Schwarz for reading the manuscript carefully and making many useful remarks, and Don Coppersmith for supplying counterexamples to the maximality of E_k which inspired Theorem 5.

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Received 11 April 1984; revised 26 April 1984